Indian J. Phys. **64A** (2), 156-159 (1990)

X-ray study of DL-lysine mono- and dihydrochloride

B Khawas
Division of Agricultural Physics, Indian Agricultural Research Institute, New Delhi-110 012, India

Received 4 December 1989, accepted 22 December 1989

The crystal structures of L-lysine HCl dihydrate (Wright and Marsh 1962) and the dimorphism of DL-lysine HCl monohydrate (Khawas 1988) were reported. So the above titled compounds, crystallised from dilute hydrochloric acid as microcrystals have been studied by taking powder patterns on a Philips X-ray diffractometer using CuK_α-radiation. The patterns were similar as reported by Parsons *et al* (1970). Possibility for higher crystal symmetries were excluded by applying Azároff and Buerger's (1958) method. The constants of analysis were obtained from differences in $\sin^2\theta$ values for orthorhombic symmetry following Lipson's (1949) method. The figure of merit calculated for the first thirty lines using Smith and Snyder's (1979) formula, indicated that the indexing was sufficiently correct.

Monohydrochloride :

The observed data with the nearest index for each line have been shown in Table 1. The unit cell has $a = 14.77(5)$, $b = 17.98(9)$, $c = 13.31(5)$ Å. The observed density is 1.37(5) gm/cc which corresponds to $Z = 16$. The probable space group is *P*222 or *Pmmm* as no systematic absences could be assigned to observed reflections.

Dihydrochloride :

The observed data with the nearest index for each line have been shown in Table 2. The unit cell has $a = 16.85(5)$, $b = 18.76(4)$, $c = 7.38(2)$ Å. The observed density is 1.24(5) gm/cc which corresponds to $Z = 8$. The probable space group is *P*222 or *Pmmm* as no systematic absences could be assigned to observed reflections.

Acknowledgment

The author is grateful to Dr A M Michael, Director IARI for his kind interest in the work.

Powder data with indices for DL-lysine monohydrochloride.

Intensity	d Å	$10^4 \sin^2\theta$ (obs)	$10^4 \sin^2\theta$ (calc)	*hkl*
12	8.950	74	74	020
18	6.680	133	134	002
5	6.010	164	165	030
3	5.654	185	182	220
12	4.762	261	261	212
50	4.660	273	273	230
8	4.444	300	301	003
55	4.140	346	346	113
30	3.942	382	378	302
25	3.887	393	397	312
100	3.495	486	486	411
17	3.459	496	493	133
85	3.419	507	508	420
35	3.368	523	519	151
25	3.323	537	535	004
15	3.257	559	562	104
8	2.992	662	659	060
20	2.951	681	679	500
16	2.909	701	697	510
10	2.862	724	720	161
5	2.810	751	753	520
8	2.759	779	780	304
70	2.705	811	812	502
20	2.684	823	821	162
8	2.663	836	836	005
5	2.610	871	868	253
17	2.565	901	902	262
40	2.539	920	925	170
4	2.375	1051	1051	620
50	2.319	1103	1102	254
10	2.216	1207	1204	006
15	2.171	1258	1263	444
5	2.101	1343	1338	560
5	2.060	1397	1396	136

Table 1. (Contd.)

Intensity	d Å	$10^4 \sin^2\theta$ (obs)	$10^4 \sin^2\theta$ (calc)	*hkl*
6	2.045	1418	1415	282
5	2.036	1430	1433	074
12	2.000	1483	1484	090
9	1.981	1511	1512	190
7	1.963	1539	1541	274
3	1.894	1653	1650	713
5	1.867	1701	1705	723
5	1.827	1777	1772	801

Table 2. Powder data with indices for DL-lysine dihydrochloride.

Intensity	d Å	$10^4 \sin^2\theta$ (obs)	$10^4 \sin^2\theta$ (calc)	*hkl*
2	9.400	67	68	$02\bar{0}$
20	8.475	83	84	200
12	5.850	173	173	130
5	5.530	194	192	201
30	5.080	230	235	230
11	4.536	288	291	140
4	4.488	294	297	301
8	4.326	317	314	311
16	4.211	334	334	400
13	4.126	348	351	410
11	4.037	364	364	321
11	3.933	383	378	041
30	3.749	422	421	050
14	3.682	438	435	002
30	3.599	458	457	340
20	3.554	470	473	112
100	3.485	488	486	430
7	3.385	518	522	500
10	3.293	547	551	151
25	3.222	571	566	341
9	3.145	600	604	440
11	3.095	619	623	302

Table 2. (Contd.)

Intensity	dÅ	$10^4 \sin^2\theta$ (obs)	$10^4 \sin^2$ (calc)	*hkl*
25	2.987	665	670	232
15	2.921	695	690	322
6	2.884	713	712	441
9	2.839	736	736	161
7	2.786	764	769	610
6	2.766	775	774	332
8	2.745	787	788	242
11	2.715	804	799	261
20	2.665	835	837	422
7	2.637	853	856	052
4	2.525	930	934	071
6	2.484	961	957	502
5	2.460	980	980	003
9	2.425	1008	1012	631
10	2.402	1028	1023	700
4	2.371	1055	1052	551
6	2.314	1108	1109	532
9	2.255	1166	1161	280
4	2.209	1215	1214	233
4	2.024	1448	1448	290
4	1.983	1508	1513	082
9	1.926	1599	1600	580
4	1.834	1763	1762	104

References

Azároff L V and Buerger M J 1958 *The podwer method in X-ray crystallography* (New York McGraw Hill) p 118

Khawas B 1988 *Indian J. Phys.* **62A** 553

Lipson H 1949 *Acta Crysta.* **2** 43

Parsons J, Scilla J A and Beher W T 1970 *Henry Ford Hosp. Med. J.* **18** 283

Smith G S and Snyder R L 1979 *J. Appl. Cryst.* **12** 60

Wright D A and Marsh R E 1962 *Acta Crysta.* **15** 54